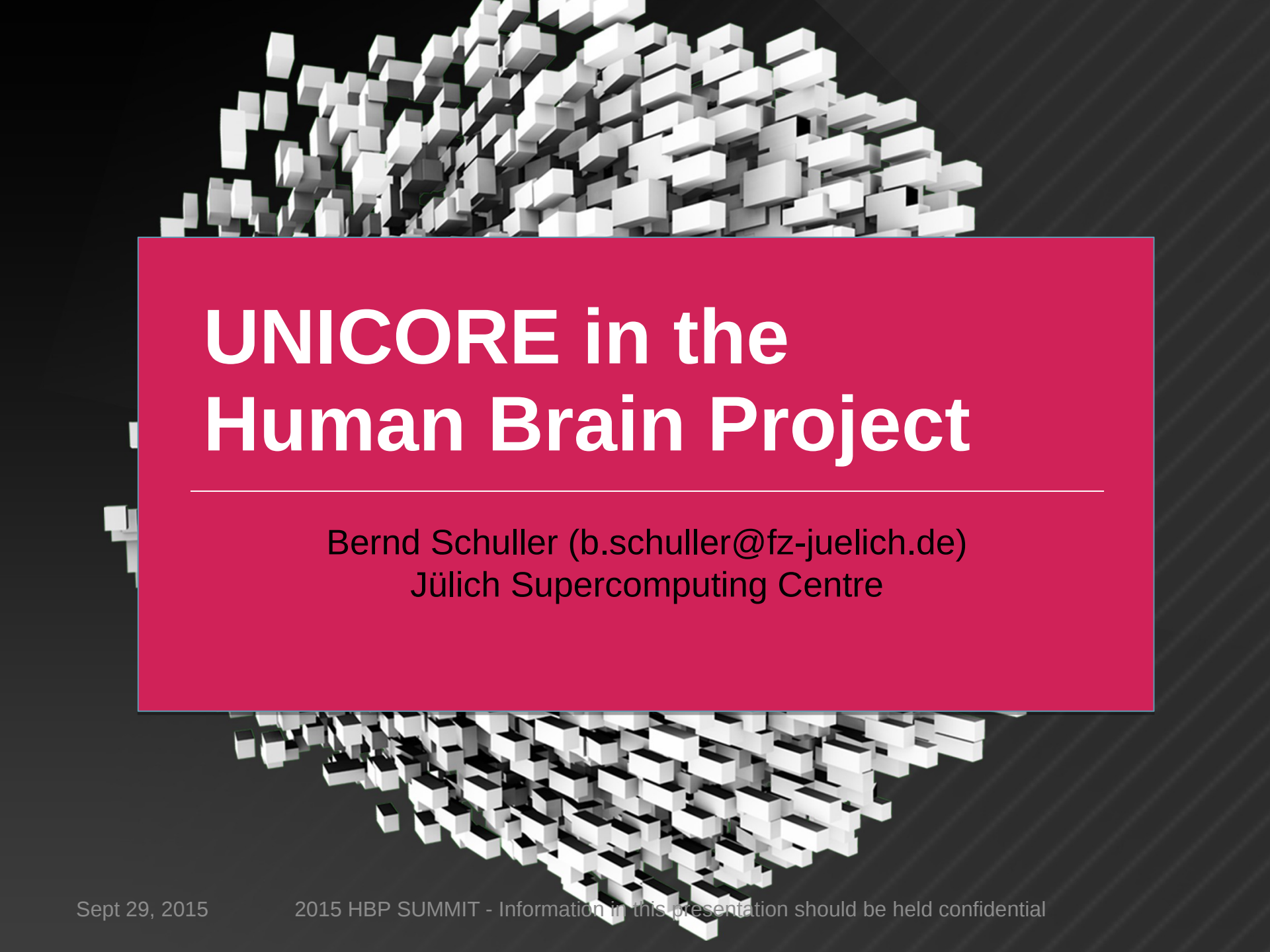
Human Brain Project

European Commission



UNICORE in the Human Brain Project

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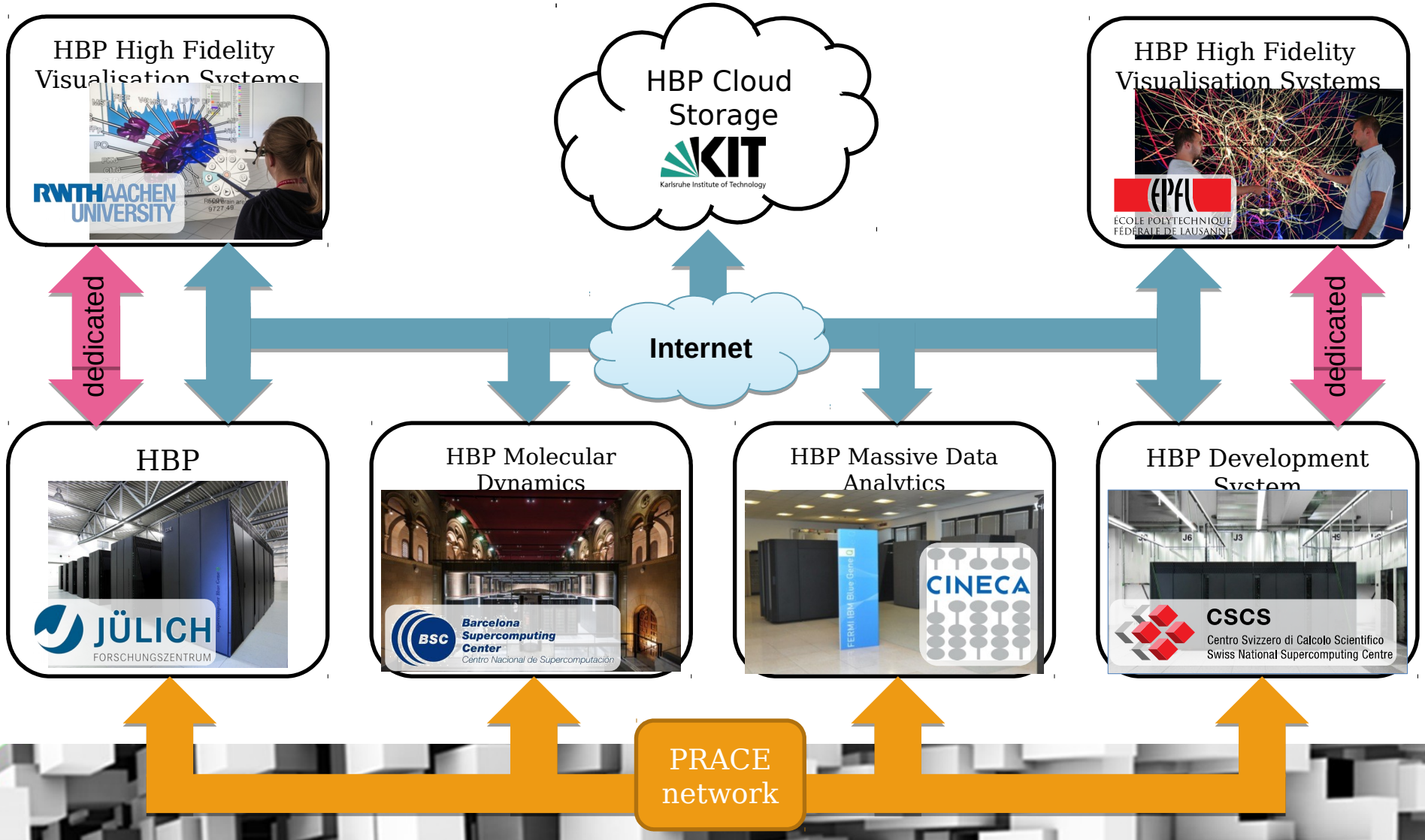
Hardware infrastructure



Systems access?

- Login/password or ssh key
- qsub, qstat, runjob, mpirun, ...
- Setting cores, nodes, memory, ...
- /usr/local/apps/myapp/bin/myapp, …
- ~/mydata/2011/job123/ergebnisse.txt, ...

ssh / scp

Systems access?

How can I ...

- … use multiple, heterogeneous systems seamlessly and securely
- … manage my job input data and results?
- … across systems? Workflows?
- ... integrate HPC/data resources into applications/portals?

UNICORE

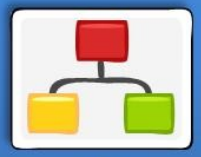

Web


Command line


GUI

API

Clients


Workflows


Jobs


Data Management


Discovery

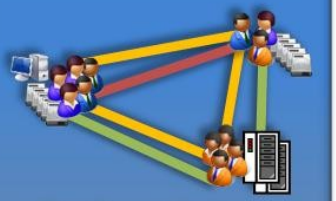
Services


Compute


Storage

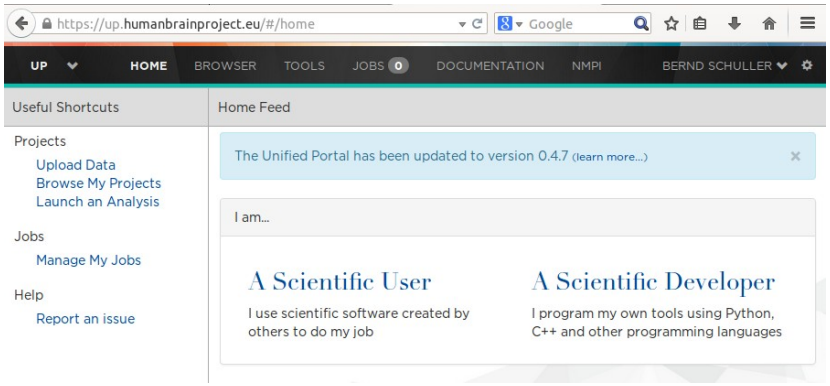
Resources


Users


Federations


Policies

Security



Collaboratory, other portals and applications

1. authenticate

returns OIDC token

OIDC server

3.1 validate OIDC

2. access REST APIs pass OIDC token

3. pass OIDC token

returns signed SAML

Unity

SOAP/WS API

REST API

UNICORE

BSC

HPC site

CINECA

HPC site

CSCS

HPC site

JSC

HPC site

KIT

S3 storage

Single sign-on

- Unity
  - Bridges UNICORE to HBP OIDC infrastructure
  - Supports REST and Web clients
  - Support for SOAP/WS clients (legacy)
- User management
  - Users are granted resources (-> review process)
  - User IDs and groups are mirrored to HPC sites (LDAP)
  - Access via UNICORE is configured automatically
- Go get an HBP account and compute time!

Running NEST - without UNICORE

- Login via ssh to JUQUEEN
- Manage working directory, code, input params
- Create/submit LoadLeveler script

```
#job_name          = slns_demo
#...
#@bg_size          = 32
#@wall_clock_limit = 00:10:00

module load python3/3.4.2
export TMPDIR=$WORK/tmp
export PYTHONPATH=/homeb/slns/slns007/local/opt/...

runjob --ranks-per-node 1 --exp-env ... : /bgsys/.../python3 microcircuit.py
```

Running NEST - using UNICORE

- Complexity is now on hidden by UNICORE
- User can use a UNICORE Application “NEST”
- User need only invoke the application and provide relevant data

```
ApplicationName: NEST,

Parameters: [
  NESTCODE: microcircuit.py, PARAMETERS: parameters.py, ],

Imports: [ ... ],

Resources: { Nodes: 32, Runtime: 1200 }
```

Running NEST - using UNICORE

- Admin defines UNICORE Application “NEST” for JUQUEEN

```
<idb:IDBApplication>

  <idb:ApplicationName>NEST</idb:ApplicationName>

  <jsdl:POSIXApplication>
    <jsdl:Executable>runjob --ranks-per-node 1 --exp-env ... : .../python3</jsdl:Executable>
    <jsdl:Argument Type="filename">$NESTCODE?</jsdl:Argument>
    <jsdl:Argument Type="filename"># $PARAMETERS?</jsdl:Argument>
  </jsdl:POSIXApplication>

  <idb:PreCommand>#@environment = COPY_ALL</idb:PreCommand>
  <idb:PreCommand>module load python3/3.4.2</idb:PreCommand>
  <idb:PreCommand>export TMPDIR=$WORK/tmp</idb:PreCommand>
  <idb:PreCommand>export PYTHONPATH=/usr/local/...:$PYTHONPATH</idb:PreCommand>

  <idb:PostCommand>find -name *gdf | xargs zip output.zip</idb:PostCommand>

</idb:IDBApplication>
```

Outlook – Collaboratory integration

- Task framework
  - THE way to integrate scientific computations into the Collaboratory
  - Autogenerated Web UI, provenance support etc
  - But: currently only uses local resources
- HPC support in the Collaboratory
  - Via UNICORE
  - OIDC support and REST API are available
  - Job submission and management is very easy
  - Data management needs to be better defined

Summary

- Secure and easy access to HPC compute and storage resources
- UNICORE provides compute and storage abstractions. Acts as integration layer for a unified view on the underlying resources
- Allows integration of HCP/Storage into custom applications using the REST API
- HBP single sign-on via OIDC supported

For more on UNICORE: http://www.unicore.eu